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Critical phenomena without "hyper scaling": How is the finite-size scaling analysis of Monte Carlo data affected?

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Abstract

The finite size scaling analysis of Monte Carlo data is discussed for two models for which hyperscaling is violated: (i) the random field Ising model (using a model for a colloid-polymer mixture in a random matrix as a representative) (ii) The Ising bi-pyramid in computing surface fields.

When one studies critical phenomena with Monte Carlo simulation, a basic obstacle always has been – and still is – the problem of finite sizes effects [1, 2]: near a critical point in the thermodynamic limit, the correlation length ξ diverges to infinity, while the simulation of a d-dimensional model system usually deals with a (hyper)cubic box of finite linear dimension L. Since a divergent correlation length does not fit into a finite box, in the simulation one can only observe a rounded and shifted transition. E.g., in the simplest case, the phase transition of the Ising ferromagnet, the distribution $P_L(m)$ of the magnetization m completely gradually changes from a double peak distribution far below the critical temperature T_c a single gaussian (centered at $m = 0$) far above T_c [1]. While far below T_c the peak positions are good estimates for $\pm m_b$, m_b being the spontaneous magnetization, near T_c this is not true: as the theory of finite size scaling shows, even right at T_c one still has a double peak distribution, but now the peaks occur at $\pm m_L$ with $m_L \propto L^{-\beta/\nu}$, where β, ν are the critical exponents $\{m_b \propto (1 - T/T_c)^{\beta}\}$[3] $\{\xi \propto |1 - T/T_c|^{-\nu}\}$. Similarly, the susceptibilities χ_+, χ_- (the sign referring to the sign of $T/T_c - 1$), estimated from the fluctuation relations $k_B T\chi_+ = L^d\langle m^2\rangle$, $k_B T\chi_- = L^d(\langle m^2\rangle - \langle|m|\rangle^2)$, reach only finite values at $T_c\{\chi_+ \propto \chi_- \propto L^{\gamma/\nu}$, where γ is the susceptibility exponent, $\chi_+ \propto \chi_- \propto |1 - T/T_c|^{-\gamma}$ in the limit $L \to \infty\}$. The temperature $T_\chi^{\max}$ where χ_- exhibits a maximum is shifted away from T_c (the same is true for the maximum of the specific heat, etc.).

However, it is well known that simulations for a series of different sizes L for the same model, and studying the size dependence using the above finite size scaling relations yield valuable information on criticality [1]. T_c can be obtained from [2] cumulant $U_L = 1 - \langle m^4\rangle/[3\langle m^2\rangle^2]$ of $P_L(m)$, since finite size scaling implies that U_L in the scaling limit is a function of L/ξ only,

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$U_L = \tilde{U}(L/\xi)$. At criticality (where $\xi = \infty$) one expects $U_L = \tilde{U}(0)$, independent of L. Such finite size scaling methods (and variants thereof) are successful and widely used; a recent example [4] concerns the adsorption of diatomic molecules (such as CO) at the (100) surface of cubic crystals; this surface provides a square lattice, at each site either a C-atom or an O-Atom or nothing gets absorbed. Allowing for nearest and next nearest neighbor interactions, many periodic superstructures occur and complicated phase diagrams result. Although then the order parameter distribution is more complicated (the order parameter may have several components) cumulant intersections do yield the phase boundaries [4].

However, there is one basic problem with the whole approach: finite size scaling relies on hyperscaling, i.e. the critical exponents must satisfy the relation $d\nu = \gamma + 2\beta$ [3]. This is seen [2] from the scaling hypothesis for $P_L(m)$ {which depends on the variables m, L and temperature T, or - alternatively $-\xi$ }

$$P_L(m) = L^x \bar{P}(mL^x, \xi/L) \quad , \quad L \to \infty, \xi \to \infty, \ \xi/L \, \text{finite} \quad , \tag{1}$$

noting that the prefactor L^x is required from the normalization $\int dm P_L(m) = 1$. The moments $\langle |m|^k \rangle$ hence become functions of ξ/L, namely [2]

$$\langle |m|^\kappa \rangle = L^{-kx} \bar{M}_k(\xi/L) \quad . \tag{2}$$

Requiring that $\langle |m| \rangle$ for $L \to \infty$ at fixed (large) ξ reduces to $m_b \propto \xi^{-\beta/\nu}$ implies that $\bar{M}_k(\varsigma) \propto (\varsigma)^{-\beta/\nu}$ and that the L-dependence cancels out, which requires that the exponent x becomes $x = \beta/\nu$. Combining this with the above fluctuation relations yield [2]

$$k_B T \chi_+ = L^d \langle m^2 \rangle = L^{d-2\beta/\nu} \bar{M}_2(\xi/L), k_B T \chi_- = L^{d-2\beta/\nu} \bar{\chi}_-(\xi/L) \tag{3}$$

with $\bar{\chi}_- = \bar{M}_2 - \bar{M}_1^2$. In order that the power laws $\chi_+, \chi_- \propto \xi^{\gamma/\nu}$ for $L \to \infty$ are reproduced, however, we need both $\bar{M}_2(\zeta)$. $\bar{\chi}_{(\zeta)} \propto \zeta^{d-2\beta/\nu}$ and $d - 2\beta/\nu = \gamma/\nu$, i.e. hyperscaling!

Now there are several cases where hyperscaling is violated: one very prominent case is the random field Ising model,(RFIM) [5, 6], and the 3-state Potts model in random field [7], etc. The hyperscaling relation is replaced by [6]

$$\gamma + 2\beta = \nu(d - \Theta), \quad \Theta = 2 - \eta = \gamma/\nu \, . \tag{4}$$

A key observation is that the RFIM has two susceptibilities, the disconnected (χ_{dis}) and the connected (χ) one [6],

$$k_B T \chi^+_{\text{dis}} = \sum_{\vec{r}} g_{\text{dis}}(\vec{r}), \ \ g_{\text{dis}}(\vec{r}) = [\langle S_o \rangle_T \langle S_{\vec{r}} \rangle_T]_{\text{av}} \quad , \tag{5}$$

$$k_B T \chi_+ = \sum_{(\vec{r})} g_{\text{conn}}(\vec{r}), \ \ g_{\text{conn}}(\vec{r}) = [\langle S_o S_r \rangle_T - \langle S_o \rangle_T \langle S_{\vec{r}} \rangle_T]_{\text{av}} \quad . \tag{6}$$

Note the double averaging: $\langle \cdots \rangle_T$ is a thermal average, $[\cdots]_{\text{av}}$ the average over the quenched random field. We now have $\chi_{\text{dis}} \propto (T/T_c - 1)^{-\gamma}$, $g_{\text{dis}}(T = T_c) \propto r^{-(d-4+\overline{\eta})}$ while $g_{\text{conn}}(T = T_c) \propto r^{-(d-2+\eta)}$, and the relations $\overline{\gamma} = \nu(4 - \overline{\eta})$, $\gamma = \nu(2 - \eta)$ and $\overline{\eta} = 2\eta$, $\overline{\gamma} = 2\gamma$ hold. These relations can also be understood [7] via finite size scaling, since $L^d[\langle m^2 \rangle]_{\text{av}}$ yields $k_B T \chi^+_{\text{dis}}$ and hence it is $\overline{\gamma}$ rather than γ that satisfies hyperscaling, $\overline{\gamma} + 2\beta = d\nu$. In fact, since in a volume L^d the random field excess of one sign of order $H_{\text{RF}} L^{-d/2}$ induces a magnetization $\langle m \rangle = \chi H_{\text{RF}} L^{-d/2}$, and using at T_c the power laws $\langle m \rangle \propto L^{-\beta/\nu}$, $\chi \propto L^{\gamma/\nu}$ one concludes that $d/2 = \beta/\nu + \gamma/\nu$, i.e. is Eq. (4) [7].

An important consequence of these observations is that the width of the peaks of $P_L(m)$ scales like $L^{(\gamma/\nu-d)/2}$ while the position scales $L^{-\beta/\nu} = L^{(2\gamma/\nu-d)/2}$: this means the distribution function $P_L(m)$ at T_c for $L \to \infty$ tends to a sum of delta functions [7]!

The first evidence for such a behavior was found for the 3-state random field Potts model [7]. Then no unique nontrivial cumulant intersection point can be found, rather the intersections converge to the $T = 0$ value [7].

This anomalous behavior of $P_L(m)$ has also been used to clarify a longstanding puzzle about the critical behavior of liquid-gas type transitions in random porous media. DeGennes [8] argued that these systems also belong to the RFIM universality class. However, previous simulations [9] and experiments [10] could not verify this prediction. Vink et al. [11] reconsidered this problem, using the Asakura Oosawa model [12] of colloid polymer mixtures. Colloids are represented as hard spheres of radius R_c, polymers as soft spheres of radius R_p (which may overlap each other, but not the colloids, and thus create an entropic force, "depletion attraction", among the colloids). One takes as a temperature-like variable the polymer fugacity z_p {or the "polymer reservoir packing fraction" $\eta_p^r = z_p(4\pi R_p^3/3))$}. Sampling the distribution $P_L(\eta_c)$ of the colloid packing fraction $\eta_c = (4\pi R_c^3(3)N_c/L^d$, N_c being the number of colloids in the box, varying the colloid chemical potential μ at fixed η_p^r is analogous to a sampling of $P_L(m)$ as functional magnetic field at fixed T for an Ising model [13]. From the equal weight rule one constructs the coexistence curve between the gas-like and liquid-like phase of this colloid dispersion [13]. The critical point then can be accurately located by the cumulant intersection, and Ising critical exponents have been verified [13].

If now a fraction of the colloids is randomly fixed in space, the resulting random porous structure creates a quenched part of the depletion force, which acts as a random field [8]. Already a very small fraction of immobile colloids leads to a strong shift of T_c and anomalously large finite size effects [11]. Defining $m = \eta_c - \eta_c^{\text{crit}}$, η_c^{crit} is the colloid packing fraction at criticality, then $U_1 \equiv [\langle m^2 \rangle_T]_{\text{av}}/[\langle |m| \rangle_T^2]_{\text{av}}$ rapidly decreases [11] from its Ising value at criticality ($U_1^* \approx 1.25$) with increasing packing fraction η_M of the particles in the frozen matrix towards $U_1^* = 1$, a value resulting if $P_L(m)$ at criticality is a sum of delta functions. Also the value of the effective exponent $(\beta/\nu)_{\text{eff}}$ displays a strong decrease towards the RFIM value (the asymptotic critical region is not reached due to crossover between the universality classes of the pure Ising model and the RFIM) [11].

Now Eq. (4) is not the only possibility for a hyperscaling violation. The most well-known case, in fact, occurs already for the Landau mean field theory [14, 15], which yields the correct critical behavior for $d > 4$, with exponents $\beta = 1/2$, $\nu = 1/2$, $\gamma = 1$ [3]. However, in this case the average magnetization of the system m dominates the behavior of $P_L(m)$, while inhomogenous fluctuations of m yield corrections only. Thus [14, 15]

$$P_L(m) \propto \exp[-L^d f_L(m)/k_BT] \quad , \tag{7}$$

where $f_L(m)$ just is nothing but the Landau free energy density

$$f_L(m) = \frac{1}{2}rm^2 + \frac{1}{4}um^4 + \cdots, r \propto (T/T_c - 1)\,. \tag{8}$$

From this ansatz one readily shows that a behavior analogous to Eq. (2) results, but with ξ being replaced by the "thermodynamic length" ℓ_T [14]

$$\langle |m|^k \rangle = L^{-kd/4} \bar{M}_K(\ell_T/L)\,,\; \ell_T \propto |T/T_c - 1|^{-2/d} \quad . \tag{9}$$

While corrections to this behavior have long been debated [16], in particular for $d = 5$, Eq. (9) captures the ultimate asymptotic behavior.

An interesting variant of Eq. (7) also occurs for a $d = 3$ system, namely the Ising bi-pyramid with "competing surface fields" (i.e., the four triangular surfaces of the upper pyramid have positive sign of the surface field H_s, while at the four lower surfaces the surface field $-H_s$ acts [17]. In this system for $T_f(H_s) < T < T_c$ the magnetization is zero, because there are two equally large domains of opposite sign, separated by an interface located in the common basal plane of the pyramids. At $T_f(H_s)$ (and in the thermodynamic limit) the interface starts to move towards one of the pyramid corners, and a spontaneous magnetization appears (this transition is related to "cone filling" in systems undergoing a condensation from gas to liquid [18].) This transition is also described by Eq. (7), but Eq. (8) gets size-dependent coefficients [17]

$$f_L(m) = \frac{1}{2L} r m^2 + \frac{1}{4uL^3} m^4 \quad , \quad r \propto (H_s - H_{\rm sc}(T))/H_{\rm sc}(T) \equiv t \quad , \tag{10}$$

where we also invoked the fact that instead of varying T at fixed H_s one can also study this transition varying H_s at fixed T ($H_{\rm sc}(T)$) being the inverse function of $T_f(H_s)$. In this case one can show that [17]

$$\langle |m|^k \rangle = \bar{M}_K(tL^2) \quad . \tag{11}$$

Simulations have shown [17] that indeed the cumulants intersect at the value $\tilde{U}(0) \approx 0.2705$ of the Landau theory [15]. However, since unlike Eq. (9) there is no power law prefactor in front of $\bar{M}_K$ in Eq. (11), the curves for $\langle |m| \rangle$ itself show a universal intersection point, at the transition point of this interface-controlled transition. This transition is particularly anomalous, since Eqs. (7), (10) imply that $P_L(m)$ at $H_{\rm sc}(T)$ has no longer any L-dependence: thus, macroscopic fluctuations occur! [17].

In conclusion, the consequences of hyperscaling violations for the finite size scaling analysis of Monte Carlo data have been elucidated. It has been shown that several distinct scenarios have to be distinguished: while in the random field case $P_L(m)$ tend towards a sum of delta functions, for systems at dimensionalities exceeding the marginal dimensions, and for some interface controlled transitions, $\ln[P_L(m)]$ is described by the Landau free energy.

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